CS190C Lec9

Resource Calculation

Overview

- Peak memory calculation
- FLOPs calculation
- What is the maximum batch size?
- What is the training time comsumption?

PART1: Peak memory calculation

For certain memory resource, how can we decide some scale of allocation?

- `batch_size`
- `max_seq_len`

We need to calculate peak memory, in order to ensure not suffering from `Cuda Out Of Memory`.

Suppose: `dtype=float32`, `d_ff` = `4d_model`, `num_heads*d_qk` = `d_model`, `d_qk=d_v`, use `SwiGLU` for FFN, use `AdamW`.

We need to calculate in 4 parts:

- Parameters of model
- Activations of model during foward process
- Gradients
- Parameters of optimizer

1. Parameters of model

We need to calculate in 3 parts:

- Input layer
- Hidden layer
- Output layer

Let: b= `batch_size` , c= `seq_len` , d= `d_model` , v= `vocab_size` , h= `num_heads` , L = `num_layers`

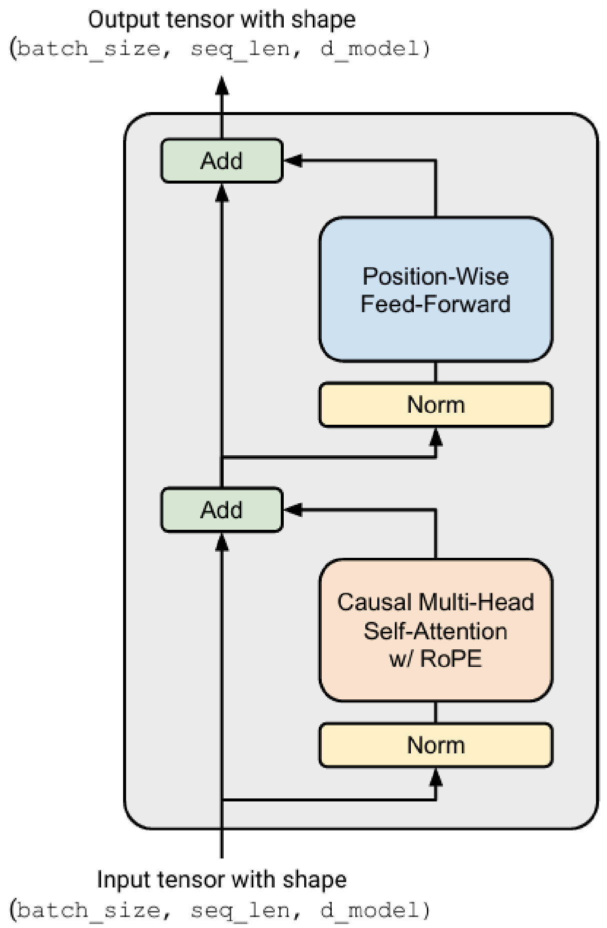
1. Parameters of model

Input layer contains word embedding matrix only:

- `vocab_size*d_model` parameters in total.

1. Parameters of model

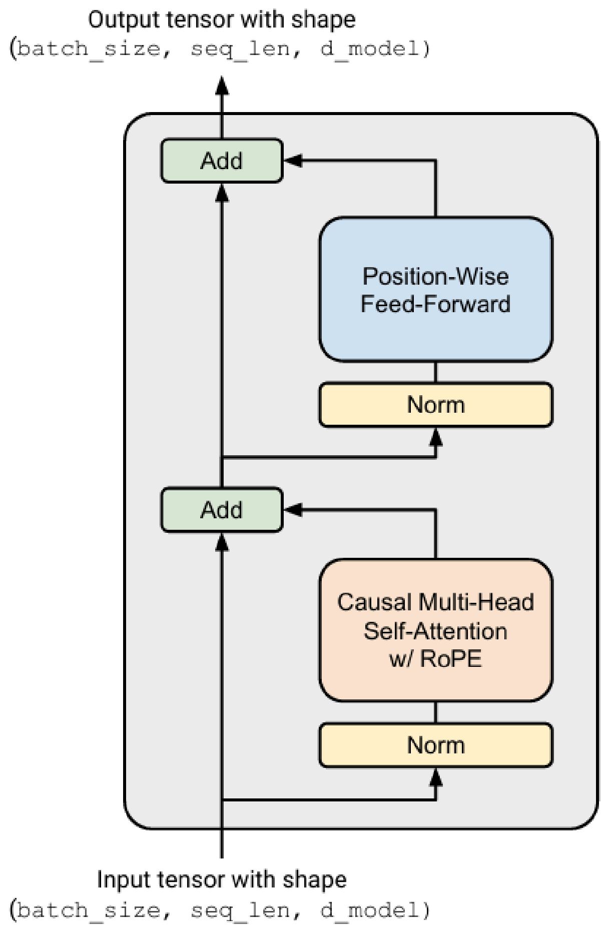
Hidden layer contains `num_layers` Transformer Blocks. For each block:


Output tensor with shape
(batch_size, seq_len, d_model)
Add
Position-Wise Feed-Forward
Norm
Add
Causal Multi-Head Self-Attention w/ RoPE
Norm
Input tensor with shape
(batch_size, seq_len, d_model)

- 2 `RMSNorm` modules: each contains `d_model` parameters, $2d$ in total.
- 1 `MHA` module:
  - W_Q,W_K,W_V: shape= `d_model*d_model` , $3d^2$ in total.
  - W_O:shape= `d_model*d_model` , $d^2 in total.
  - $4d^2$ in total.

1. Parameters of model

Hidden layer contains `num_layers` Transformer Blocks. For each block: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- 1 `FFN` module:
  - W_1: `d_model*d_ff` = `4*d_model*d_model`
  - W_3: `d_model*d_ff` = `4*d_model*d_model`
  - W_2: `d_ff*d_model` = `4*d_model*d_model`
  - $12d^2$ in total
- $L(2d + 16d^2)$ in total

1. Parameters of model

Output layer contains Final `RMSNorm` and a `Linear Projection` module.

- Final `RMSNorm`: `d_model` parameters
- `Linear Projection`: `d_model*vocab_size` parameters
- $d + dv$ in total

1. Parameters of model

Total memory of this part:

- Input layer: `vocab_size*d_model`
- Hidden layer: `num_layers*(2*d_model+16*d_model*d_model)`
- Output layer: `d_model` + `d_model*vocab_size`
- Total parameter: $N_p = 2dv + d + L(2d + 16d^2)$
- Total memory: $4 * N_p$ bytes

2. Activations of model during foward process

We should consider following modules:

- Transformer Blocks
  - Activations of `RMSNorm`s
  - Activations of `Multi-Head Attention`
  - Activations of `FFN`
- Final `RMSNorm`
- Logits of `Linear Projection` (output embeddings)

2. Activations of model during foward process

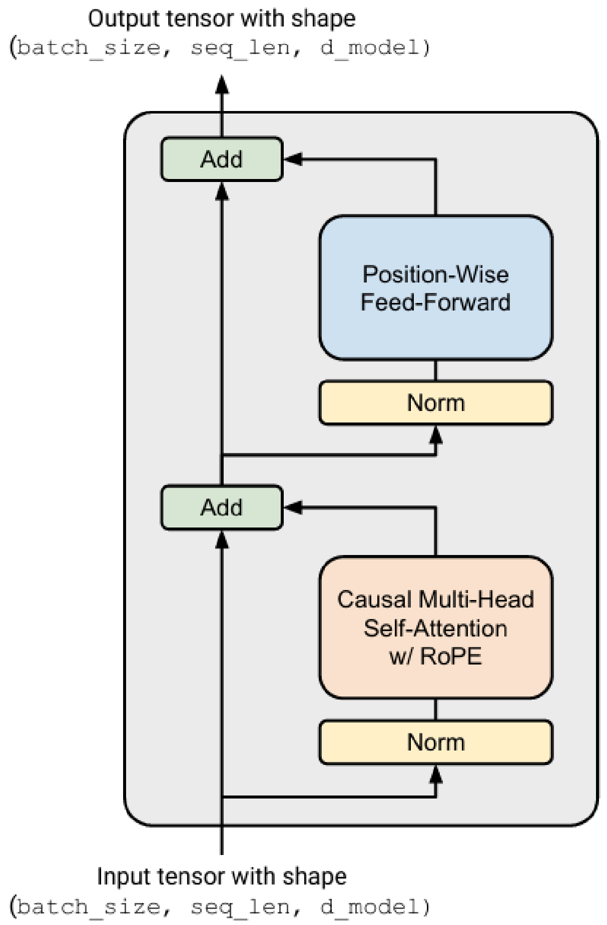
Why we need to save activations, instead of discard it right after calculated?

- We need to backward and calculate gradients after forward completed.
- Gradient calculation is related to activations!
- So we should infer what to save according to gradient calculation.

So how do we deriviate what activation to save?

- Related to backward: Nodes on the computation graph.
- Related to parameter optimization.

2. Activations of model during foward process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Input tensor with shape
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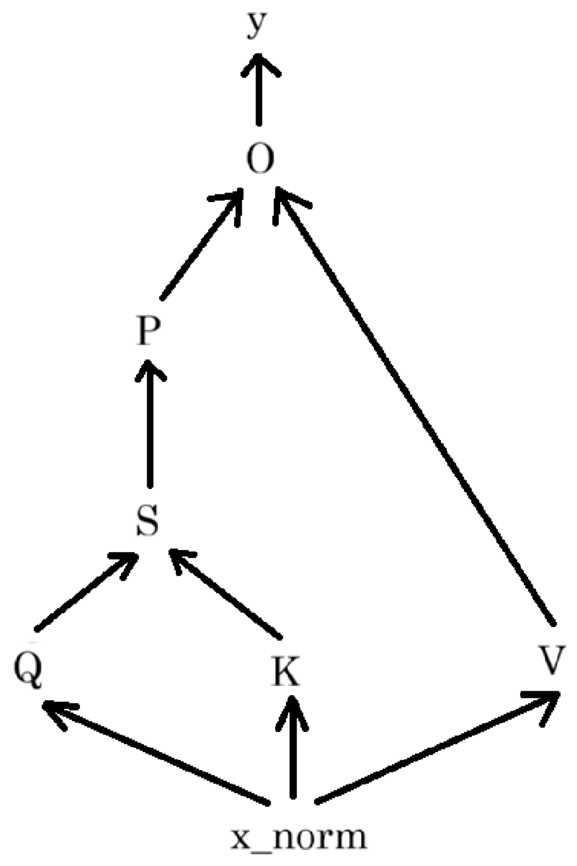
For `RMSNorm` before `MHA`:

- Forward: $x_{norm} = \frac{x}{\sqrt{\text{RMS}(x)}} \cdot g$
- Gradients calculation:
  - Gradients to calculate for backward: $\frac{\partial L}{\partial x} = \frac{\partial L}{\partial x_{norm}} \frac{\partial x_{norm}}{\partial x}$
  - Gradients to calculate for optimization: $\frac{\partial L}{\partial g} = \frac{\partial L}{\partial x_{norm}} \frac{\partial x_{norm}}{\partial g}$
- Activations to save:
  - $\frac{\partial x_{norm}}{\partial x} = f(x, g)$, containing x (g has been considered in model parameters)
  - $\frac{\partial x_{norm}}{\partial g} = \frac{x}{\sqrt{\text{RMS}(x)}}$, containing x

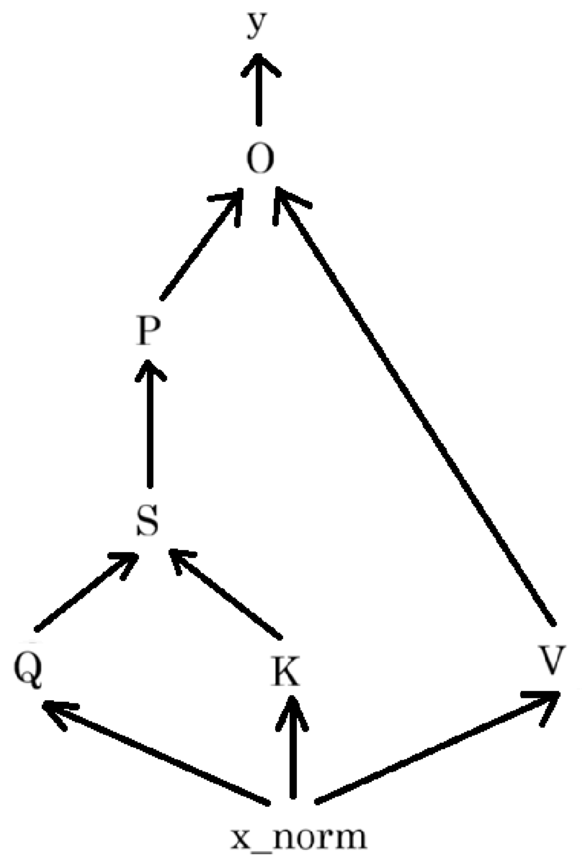
2. Activations of model during foward process



For calculation of `Q` `K` `V` in `MHA`:

- Forward: $Q = W_Q x_{norm}$, K, V the same.
- Gradients calculation:
  - Gradients to calculate for backward:
    $$\frac{\partial L}{\partial x_{norm}} = \frac{\partial L}{\partial Q}\frac{\partial Q}{\partial x_{norm}} + \frac{\partial L}{\partial K}\frac{\partial K}{\partial x_{norm}} + \frac{\partial L}{\partial V}\frac{\partial V}{\partial x_{norm}}$$
  - Gradients to calculate for optimization:
    $\frac{\partial L}{\partial W_Q} = \frac{\partial L}{\partial Q}\frac{\partial Q}{\partial W_Q}$, W_Q, W_K the same.
- Activations to save:
  - $\frac{\partial Q}{\partial x_{norm}} = W_Q$, has been considered.
  - $\frac{\partial Q}{\partial W_Q} = x_{norm}$.
  - Save x_{norm}.

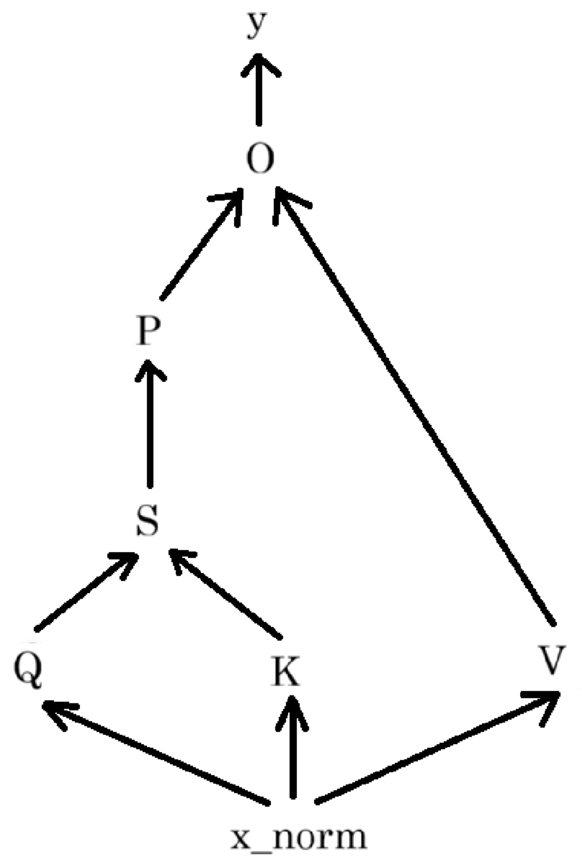
2. Activations of model during foward process


$$\begin{tikzcd} & & y & \\ & & O \arrow[u] & \\ & P \arrow[ur] & & \\ & S \arrow[u] & & \\ Q \arrow[ur] & & K \arrow[ul] & V \arrow[uuull] \\ & & x\_norm \arrow[ull] \arrow[u] \arrow[ur] & \end{tikzcd}$$

For calculation of Attention Score `S` in `MHA`:

- Forward: $S = \frac{Q^T K}{\sqrt{d_k}}$
- Gradients calculation:
    - Gradients to calculate for backward: $\frac{\partial L}{\partial Q} = \frac{\partial L}{\partial S} \frac{\partial S}{\partial Q}, \frac{\partial L}{\partial K}$ is the same.
    - No learnable parameters.
- Activations to save:
    - $\frac{\partial S}{\partial Q} = K, \frac{\partial S}{\partial K} = Q$
    - Save `Q`, `K`
- Shape: `[bsz,seq_len,d_model]`; Numbers: $2bcd$

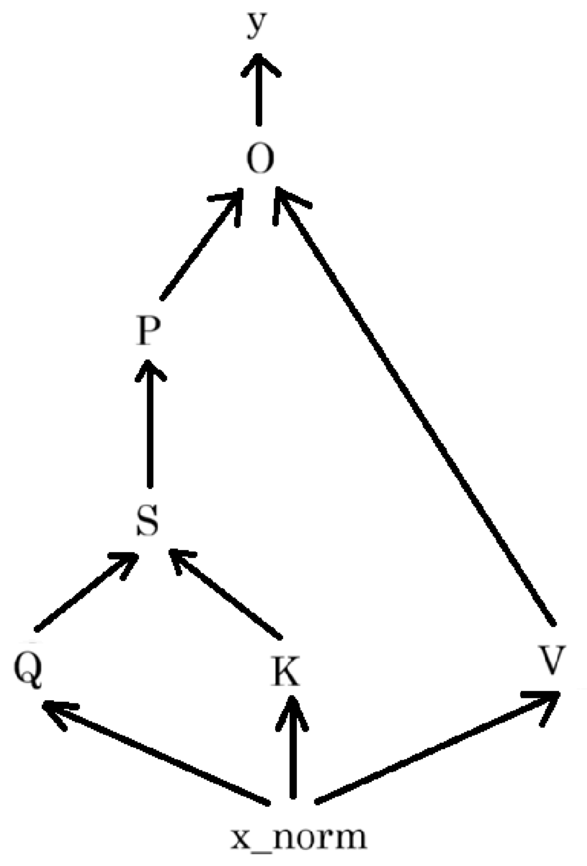
2. Activations of model during foward process



For calculation of Attention Weight `P` in `MHA`:

- Forward: $P = \mathrm{Softmax}(S)$
- Gradients calculation:
  - Gradients to calculate for backward: $\frac{\partial L}{\partial S} = \frac{\partial L}{\partial P} \frac{\partial P}{\partial S}$
  - No learnable parameters.
- Activations to save:
  - $\frac{\partial P}{\partial S} = f(P)$
  - Save `P`
- Shape: `[bsz,num_heads,seq_len,seq_len]`; Numbers: bhc^2

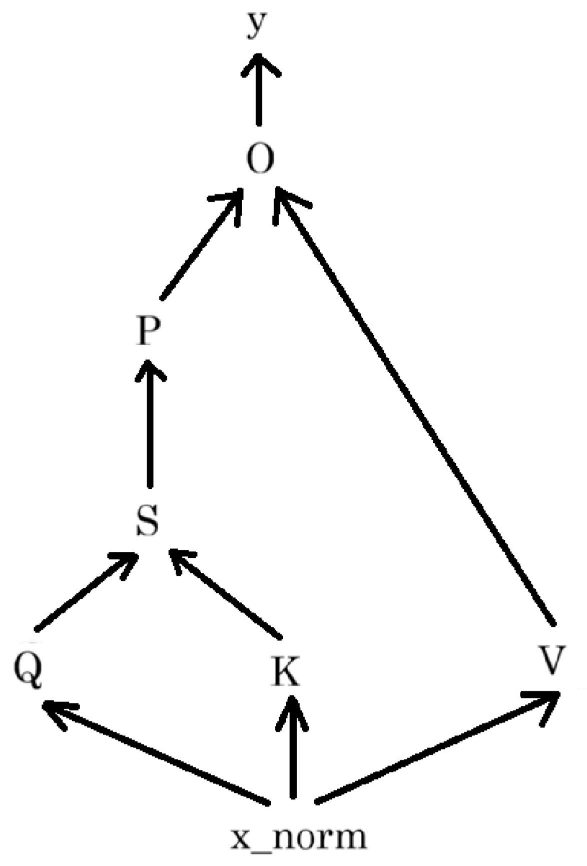
2. Activations of model during foward process



For calculation of multi-head output `O` in `MHA`:

- Forward: $O = PV$
- Gradients calculation:
  - Gradients to calculate for backward: $\frac{\partial L}{\partial P} = \frac{\partial L}{\partial O}\frac{\partial O}{\partial P}$, V is the same.
  - No learnable parameters.
- Activations to save:
  - $\frac{\partial O}{\partial P} = V$, $\frac{\partial O}{\partial V} = P$
  - Save `V` (`P` has been saved)
- Shape: `[bsz,seq,d_model]`; Numbers: bcd

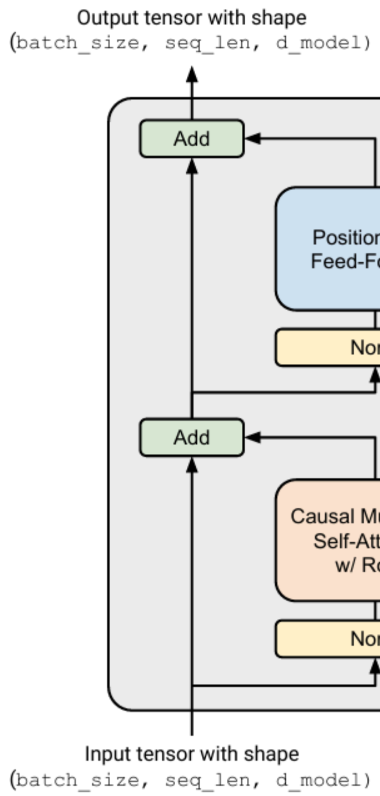
2. Activations of model during foward process



For calculation of attention output `y` in `MHA`:

- Forward: $y = W_O O$
- Gradients calculation:
  - Gradients to calculate for backward: $\frac{\partial L}{\partial O} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial O}$
  - Gradients to calculate for optimization: $\frac{\partial L}{\partial W_O} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial W_O}$
- Activations to save:
  - $\frac{\partial y}{\partial O} = W_O$ (has been saved)
  - $\frac{\partial y}{\partial W_O} = O$
  - Save `O`

2. Activations of model during foward process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Input tensor with shape
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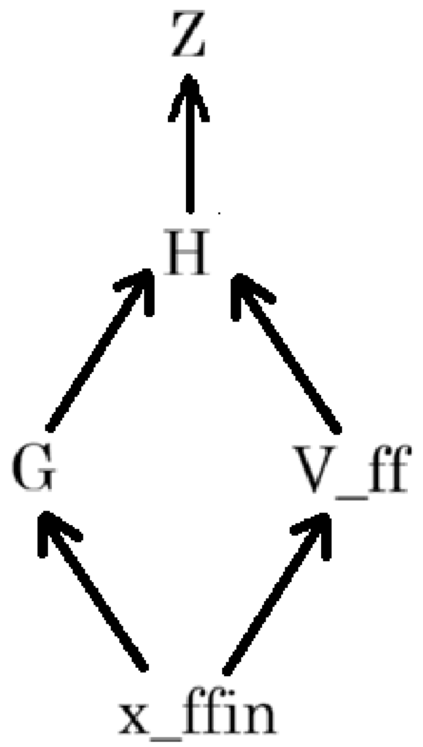
For residual connection and `RMSNorm` before `FFN`:

- Forward: $x_{res} = x + y$, $x_{ffin} = \frac{x_{res}}{\sqrt{\mathrm{RMS}(x_{res})}} \cdot g_2$
- Gradients calculation:
  - Gradients to calculate for backward:
    $$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial x_{ffin}} \frac{\partial x_{ffin}}{\partial x_{res}} \frac{\partial x_{res}}{\partial y}$$
  - Gradients for g_2
- Activations to save:
  - Save `x_res`
- Shape: `[bsz,seq,d_model]`; Numbers: bcd

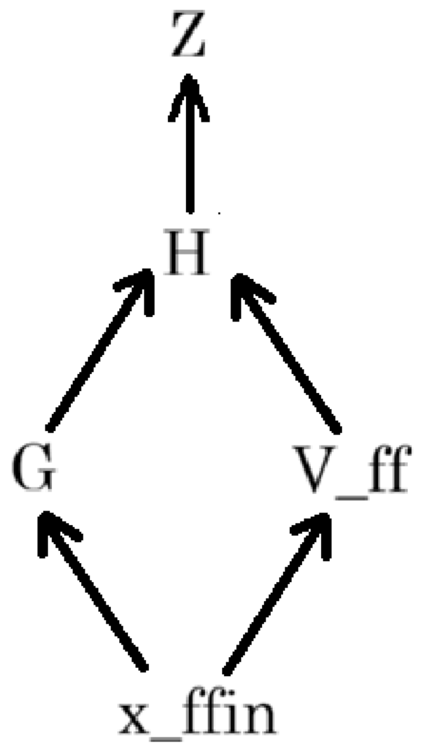
2. Activations of model during foward process



For W1 Gate in `FFN`:

- Forward: $G = W_1 x_{ffin}$
- Gradients calculation:
  - Gradients to calculate for backward: $\frac{\partial L}{\partial x_{ffin}} = \frac{\partial L}{\partial G} \frac{\partial G}{\partial x_{ffin}}$
  - Gradients to calculate for optimization: $\frac{\partial L}{\partial W_1} = \frac{\partial L}{\partial G} \frac{\partial G}{\partial W_1}$
- Activations to save:
  - $\frac{\partial G}{\partial x_{ffin}} = W_1$ (has been saved)
  - $\frac{\partial G}{\partial W_1} = x_{ffin}$
  - Save `x_ffin`

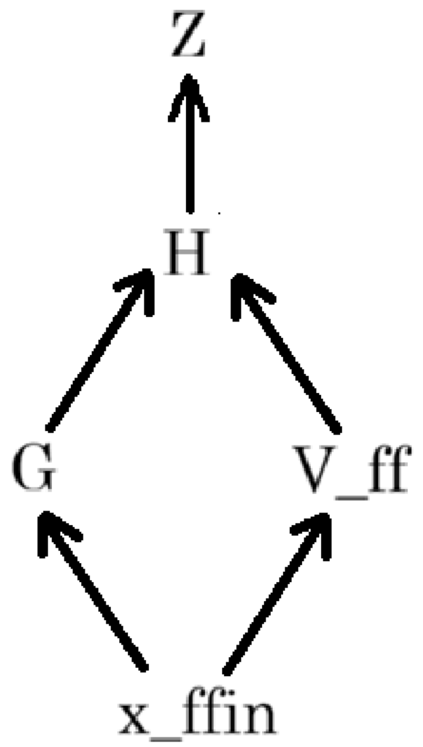
2. Activations of model during foward process



For W3 Gate in `FFN`:

- Forward: $V_{ff} = W_3 x_{ffin}$
- Gradients calculation:
  - Gradients to calculate for backward: $\frac{\partial L}{\partial x_{ffin}} = \frac{\partial L}{\partial V_{ff}} \frac{\partial V_{ff}}{\partial x_{ffin}}$
  - Gradients to calculate for optimization: $\frac{\partial L}{\partial W_3} = \frac{\partial L}{\partial V_{ff}} \frac{\partial V_{ff}}{\partial W_3}$
- Activations to save:
  - $\frac{\partial V_{ff}}{\partial x_{ffin}} = W_3$ (has been saved)
  - $\frac{\partial V_{ff}}{\partial W_3} = x_{ffin}$ (has been saved)
  - Do not need to save anything.

2. Activations of model during foward process

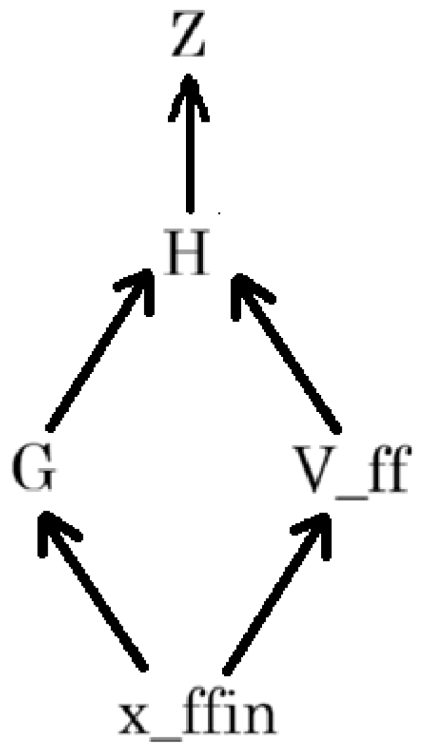


$$\begin{tikzcd} & Z & \\ & H \arrow[u] & \\ G \arrow[ur] & & V\_ff \arrow[ul] \\ & x\_ffin \arrow[ul] \arrow[ur] & \end{tikzcd}$$

For gate interaction in `FFN`:

- Forward: $H = \mathrm{SiLU}(G) \cdot V_{ff} = G \cdot \sigma(G) \cdot V_{ff}$
- Gradients calculation:
  - Gradients to calculate for backward: $\frac{\partial L}{\partial V_{ff}} = \frac{\partial L}{\partial H}\frac{\partial H}{\partial V_{ff}}, \quad \frac{\partial L}{\partial G} = \frac{\partial L}{\partial H}\frac{\partial H}{\partial G}$
  - No learnable parameters.
- Activations to save:
  - $\frac{\partial H}{\partial V_{ff}} = \mathrm{SiLU}(G)$
  - $\frac{\partial H}{\partial G} = f(G, V_{ff})$
  - Save `G`, `V_ff`
- Shape: `[bsz,seq,d_ff]`; Numbers: $8bcd$

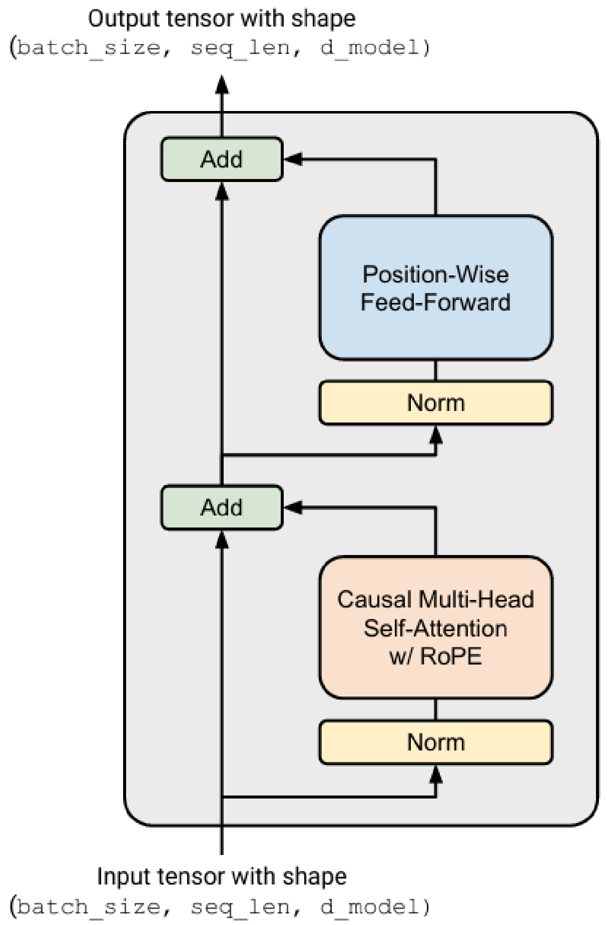
2. Activations of model during foward process



For W2 Gate in `FFN`:

- Forward: $Z = W_2 H$
- Gradients calculation:
  - Gradients to calculate for backward: $\frac{\partial L}{\partial H} = \frac{\partial L}{\partial Z}\frac{\partial Z}{\partial H}$
  - Gradients to calculate for optimization: $\frac{\partial L}{\partial W_2} = \frac{\partial L}{\partial Z}\frac{\partial Z}{\partial W_2}$
- Activations to save:
  - $\frac{\partial Z}{\partial H} = W_2$ (has been saved)
  - $\frac{\partial Z}{\partial W_2} = H$
  - Save `H`
- Shape: `[b, s, d_ff]`; Numbers: $4bsd$

2. Activations of model during foward process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Input tensor with shape
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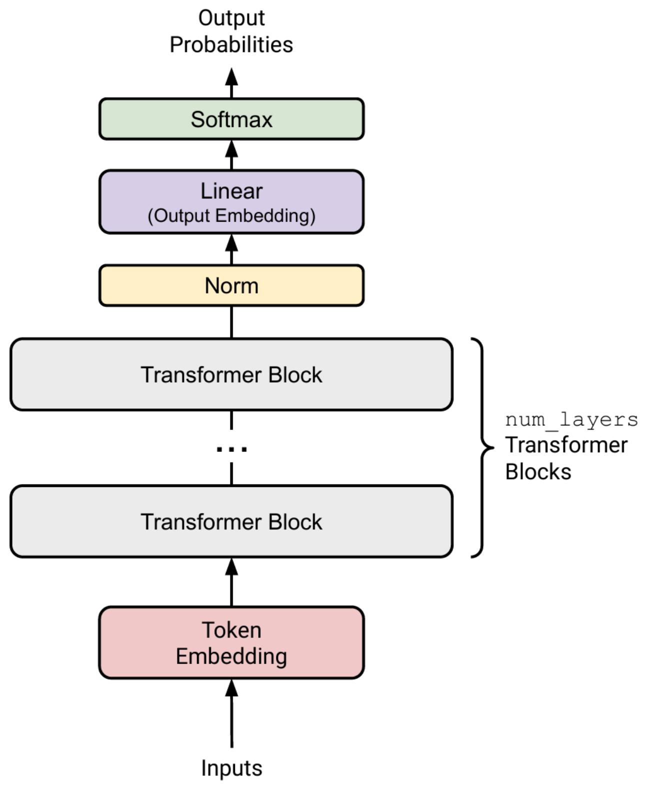
For final residual:

- Forward: $x_{out} = x_{res} + Z$
- Gradient portion=1, no learnable parameters
- No need to save anything.

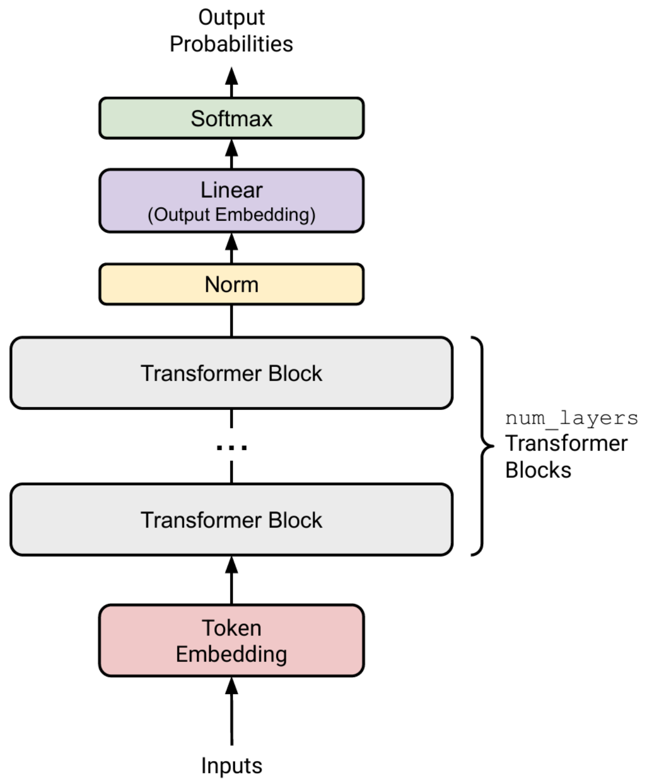
2. Activations of model during foward process



For Final `RMSNorm`:

- Forward:$X_{final} = \frac{x_{final}}{\sqrt{\text{RMS}(x_{final})}} \cdot g_{final}$
- Similarly, save the input of `RMSNorm`, that is the output of the last layer of Transformer.
- Shape: `[bsz,seq,d_model]`; Numbers: bcd

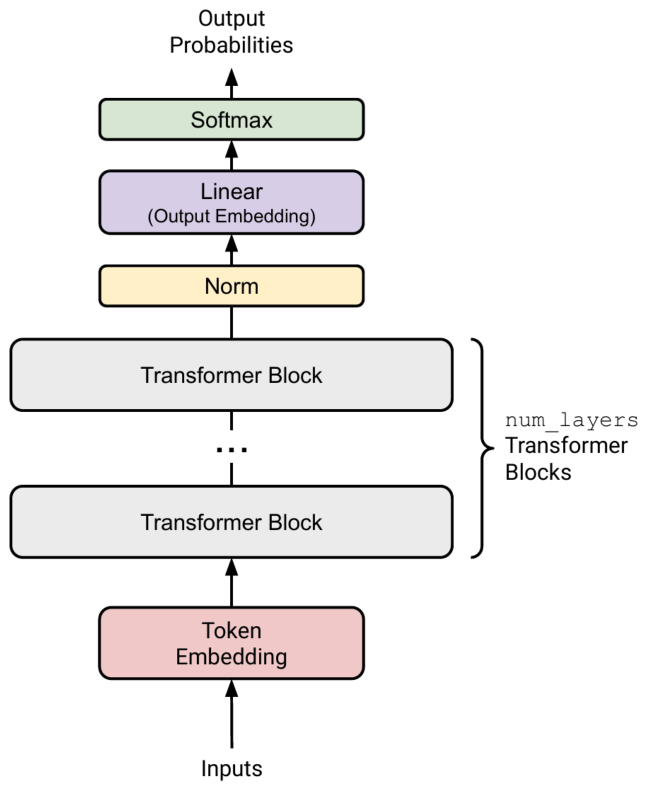
2. Activations of model during foward process



For `Output Embedding`:

- Forward: $\text{Logits} = W_{vocab} X_{final}$
- Gradients calculation:
  - Gradients to calculate for backward: $\frac{\partial L}{\partial X_{final}} = \frac{\partial L}{\partial \text{Logits}} \frac{\partial \text{Logits}}{\partial X_{final}}$
  - Gradients to calculate for optimization: $\frac{\partial L}{\partial W_{vocab}} = \frac{\partial L}{\partial \text{Logits}} \frac{\partial \text{Logits}}{\partial W_{vocab}}$
- Activations to save:
  - $\frac{\partial \text{Logits}}{\partial X_{final}} = W_{vocab}$ (has been saved)
  - $\frac{\partial \text{Logits}}{\partial W_{vocab}} = X_{final}$
  - Save `X_final`

2. Activations of model during foward process



For `Output Embedding`:

- Forward: $L = CE(\text{Logits}, \text{Standard})$
- Gradients calculation:
    - Gradients to calculate for backward: $\frac{\partial L}{\partial \text{Logits}}$
    - No learnable parameters.
- Activations to save:
    - $\frac{\partial L}{\partial \text{Logits}} = f(\text{Logits})$
    - Save `Logits`
- Shape: `[bsz,seq,vocab_size]`; Numbers: bcv

2. Activations of model during foward process

- For each Transformer Block: $20bcd + bhc^2 = N_B$ in total.
- For the whole transformer: $L * N_B + 2bcd + bcv = N_A$ in total.
- $4 * N_A$ bytes in total.

3. Gradients

It's easy: The number of elements of gradients is the same as model parameter's elements.

So $4 * N_p$ bytes in total

4. Parameters of optimizer

Parameters of AdamW:

- m_t: historical gradient $\Rightarrow$ the shape is the same as model gradients.
- V_t: historical gradient fluctuation $\Rightarrow$ the shape is the same as model gradients.

So $2 * 4 * N_p = 8 * N_p$ in total.

Peak memory calculation

The peak memory is: $16 * N_p + 4 * N_A$

$N_p = 2dv + d + L(2d + 16d^2)$

$N_A = L * N_B + 2bcd + bcv$

$N_B = 20bcd + bhc^2$

So the peak memory is:

$$\begin{aligned} &16[2dv + d + L(2d + 16d^2)] + 4[L(20bcd + bhc^2) + 2bcd + bcv] \\ &\qquad = L\left(256d^2 + 32d + 80bcd + 4bhc^2\right) + (32dv + 16d + 8bcd + 4bcv) \end{aligned}$$

PART2: FLOPs calculation

FLOPs: `Floating Point Operations`, which is use to measure how many computing resources will be comsumed.

For example: $y = AB, A \in R^{n*m}, B \in R^{m*k}$

- For each element y_{ij}: m multiples & $m - 1$ adds
- $m(nk)$ multiples and $(m-1)(nk)$ adds, approximately $2mnk$ FLOPs.

How many FLOPs for a single training iteration?

- FLOPs for a forward pass
- FLOPs for a backward pass
- FLOPs for an optimizer update pass

We mainly focus on **matrix calculation**, and neglect element-wise computation of `RMSNorm`, `Softmax` and so on.

1. FLOPs for a forward pass

For `MHA` module:

- Calculation of `Q` `K` `V`:
  - `W_QKV:[d,d]` `x:[b,c,d]`
  - FLOPs: $3b(2cdd) = 6bcd^2$
- Calculation of QK^T:
  - `Q:[b,h,c,d/h]` `K^T:[b,h,d/h,c]`
  - FLOPs: $bh(2ccd/h) = 2bc^2d$

1. FLOPs for a forward pass

For `MHA` module:

- Calculation of $\mathrm{Softmax} \cdot V = \mathrm{Attn} \cdot V$
  - `Attn:[b,h,c,c]` `V:[b,h,c,d/h]`
  - FLOPs: $bh(2ccd/h) = 2bc^2d$
- Calculation of O:
  - `Attn·V:[b,c,d]` `W_O:[d,d]`
  - FLOPs: $2bcd^2$
- In total: $8bcd^2 + 4bc^2d$

1. FLOPs for a forward pass

For `FFN` module:

- `W1` and `W3` projections:
  - `input:[b,c,d]` `proj:[b,c,4d]`, 2 projections
  - FLOPs: $2(8bcd^2) = 16bcd^2$
- `W2` projection:
  - `input:[b,c,4d]` `proj:[b,c,d]`
  - FLOPs: $8bcd^2$
- In total: $24bcd^2$

1. FLOPs for a forward pass

For a single Transformer Block:

- $32bcd^2 + 4bc^2d$ FLOPs in total
- $L(32bcd^2 + 4bc^2d)$ FLOPs for all blocks.

1. FLOPs for a forward pass

For output layer:

- `input:[b,c,d]` `proj:[d,v]`
- FLOPs: $2bcdv$

So $F_{forward} = L(32bcd^2 + 4bc^2d) + 2bcdv$ in total.

2. FLOPs for a backward pass

We only need to estimate it roughly.

For matrix calculation $Y = XW$, X is the activation, a part of the computation graph, W is the learnable parameter.

For backward:

- We need to calculate $\frac{\partial L}{\partial X} = \frac{\partial L}{\partial Y}\frac{\partial Y}{\partial X}$ (discussed in part 1.2), that is to calculate $\frac{\partial L}{\partial Y}W^T$
- We also need to calculate $\frac{\partial L}{\partial W} = \frac{\partial L}{\partial Y}\frac{\partial Y}{\partial W}$, that is to calculate $\frac{\partial L}{\partial Y}X$

The sum of FLOPs of them is roughly equals to $2F_{forward}$ (1 matrix calculation is correspond to 2)

3. FLOPs for an optimizer update pass

For AdamW:

- $m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$
  - For each element: 2 multiplications, 1 addition.
  - 3 FLOPs for each element.
- $v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$
  - For each element: 3 multiplications, 1 addtion.
  - 4 FLOPs for each element.
- $\theta_t = \theta_{t-1} - \alpha \frac{m_t}{\sqrt{v_t} + \epsilon}$
  - For each element: $\sqrt{v_t}$, $+\epsilon$, $\frac{m_t}{\sqrt{v_t}+\epsilon}$, $\alpha \frac{m_t}{\sqrt{v_t}+\epsilon}$, $\theta_{t-1} - \alpha \frac{m_t}{\sqrt{v_t}+\epsilon}$
  - 5 FLOPs for each element

3. FLOPs for an optimizer update pass

For AdamW:

- $\theta_t = \theta_t - \alpha\lambda\theta_{t-1}$
    - For each element: 2 multiplications, 1 addition.
    - 3 FLOPs for each element
- In total: $3 + 4 + 5 + 3 = 15$ FLOPs for each element
- Number of element is the number of model parameters $N_p = 2dv + d + L(2d + 16d^2)$
- $F_{optimize} = 15N_p = 30dv + 15d + 15L(2d + 16d^2)$

FLOPs calculation

FLOPs for a complete training iteration:

$$F_{total} = F_{forward} + F_{backwawrd} + F_{optimize}$$

$$= 3F_{forward} + F_{optimize}$$

$$= 3L(32bcd^2 + 4bc^2d) + 6bcdv + 30dv + 15d + 15L(2d + 16d^2)$$

PART3: What is the maximum batch size?

Suppose we have only 1 rtx3090. What the maximum batch size we can allocate without gradient accumulation?

$M_{peak} = [L(256d^2 + 32d) + (32dv + 16d)] + b[L(80cd + 4hc^2) + (8cd + 4cv)]$
=$M_{static} + bM_{per\_sample}$

$M_{3090} = 24GB = 24 * 1024^3$

$\Rightarrow b_{max} \approx \lfloor \frac{M_{3090} - M_{static}}{M_{per\_sample}} \rfloor$

$\Rightarrow b_{max} \approx \frac{24 \times 10^9 - (256Ld^2 + 32dv)}{4Lc(20d + hc)}$

PART4: What is the training time comsumption?

Suppose we have 4 rtx3090, using `wikitext103` dataset to train 5 epochs. What the time comsumption, neglecting time of evaluation?

Can we calculate like this?

$$T_{seconds} = \frac{\text{Total FLOPs}}{\text{Peak efficiency of GPU}}$$

We should consider `Model FLOPs Utilization` (MFU) of GPU. That is: GPUs are expected to work at efficiency $\text{MFU} * \text{Peak}$

$$T_{seconds} = \frac{\text{Total FLOPs}}{\text{MFU} * \text{Peak}}$$

$$\text{Total FLOPs} = \text{Total Steps} * \text{FLOPs per Step}$$

$$\text{Total Steps} * bc = \text{Total Tokens} * \text{epoch}$$

$$\Rightarrow \text{Total Steps} = \frac{5 * \text{Total Tokens}}{bc} = \frac{5.15 * 10^8}{bc}$$

$$\text{Total FLOPs} = \frac{5.15 * 10^8}{bc}(3L(32bcd^2 + 4bc^2 d) + 6bcdv + 30dv + 15d + 15L(2d + 16$$

$$T_{seconds} = \frac{5.15 * 10^8}{1.424 * 10^{14}} \frac{3L(32bcd^2 + 4bc^2 d) + 6bcdv + 30dv + 15d + 15L(2d + 16d}{bc * \text{MFU}}$$

$$T_{seconds} = 3.617 * 10^{-6} \cdot \frac{3L(32bcd^2 + 4bc^2 d) + 6bcdv + 30dv + 15d + 15L(2d + 16d^2)}{bc * \text{MFU}}$$

Suppose $b = 4, c = 256, d = 1024, L = 12, v = 32000, \mathrm{MFU} = 0.5$

$$T_{seconds} = 3.617 * 10^{-6} \cdot \frac{3L(32bcd^2 + 4bc^2d) + 6bcdv + 30dv + 15d + 15L(2d + 16d^2)}{bc * \mathrm{MFU}}$$

$$\Rightarrow T_{seconds} = 10461.9974$$

$$\Rightarrow T_{hours} = 2.9061$$